Agenda: Complex Processes in Nature and Laboratory

Systems and dynamics, qualifiers
- Examples (climate, planetary motion),

Order and Chaos, determinism and stochastic unpredictability
- 1D dynamics: phase space curves/orbits

Non-linear dynamics in nature and their modeling
- Mathematical model (logistic map, climate,…..)
- Stability criteria, stationary states

Self organizing (cooperative) processes & resulting structures
- Self-organization/replication in coupled chemical rxns
- Cellular automata and fractal structures

Dynamics of interacting multi-particle systems
- Interaction energies
- Random walk and diffusion,
- Fluctuating (Langevin) forces
- Boltzmann molecular chaos

Reading Assignments
Weeks 2&3

LN I.5-I-6: Complex processes

Kondepudi Ch.19
Additional Material
J.L. Schiff:
Cellular Automata,
Ch.1, Ch. 3.1-3.6

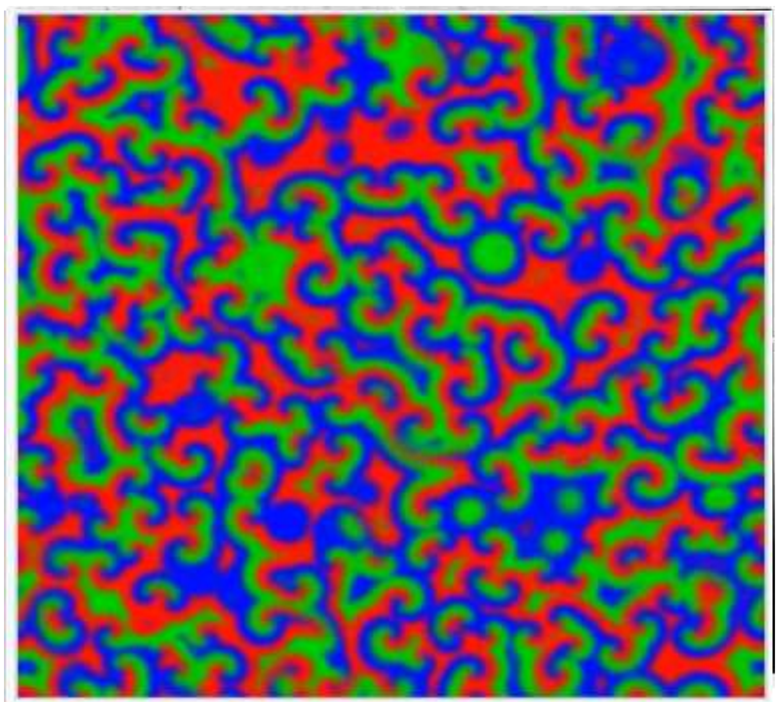
McQuarrie & Simon
Math Chapters
MC B, C, D,

Cooperative Belousov-Zhabotinski (BZ) Reaction

Oxidation of malonic acid with cerium bromate, $CeBr_3$ (*Kondepudi&Prigogine Ch. 19*)

$$2BrO_3^- + 3CH_2(COOH)_2 + 2H^+ \rightarrow 2BrCH(COOH)_2 + 3CO_2 + 4H_2O$$

→ Spatially correlated colored traveling domain patterns on reactor surface.

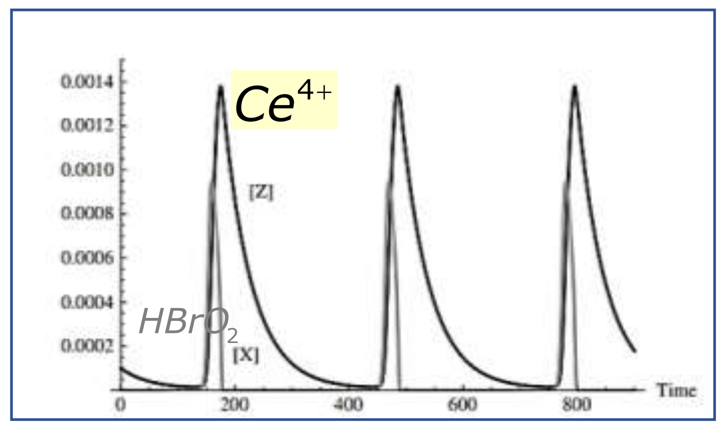


Ce = catalyst, [Ce] ≈ const., but oscillations between Ce^{3+} and Ce^{4+}, → alternating colors.

Intermediate reaction step

$$BrO_2^{\bullet} + Ce^{3+} + H^+ \rightarrow HBrO_2 + Ce^{4+}$$

(Radical)



$Ce^{3+} \rightarrow Ce^{4+}$ oscillations

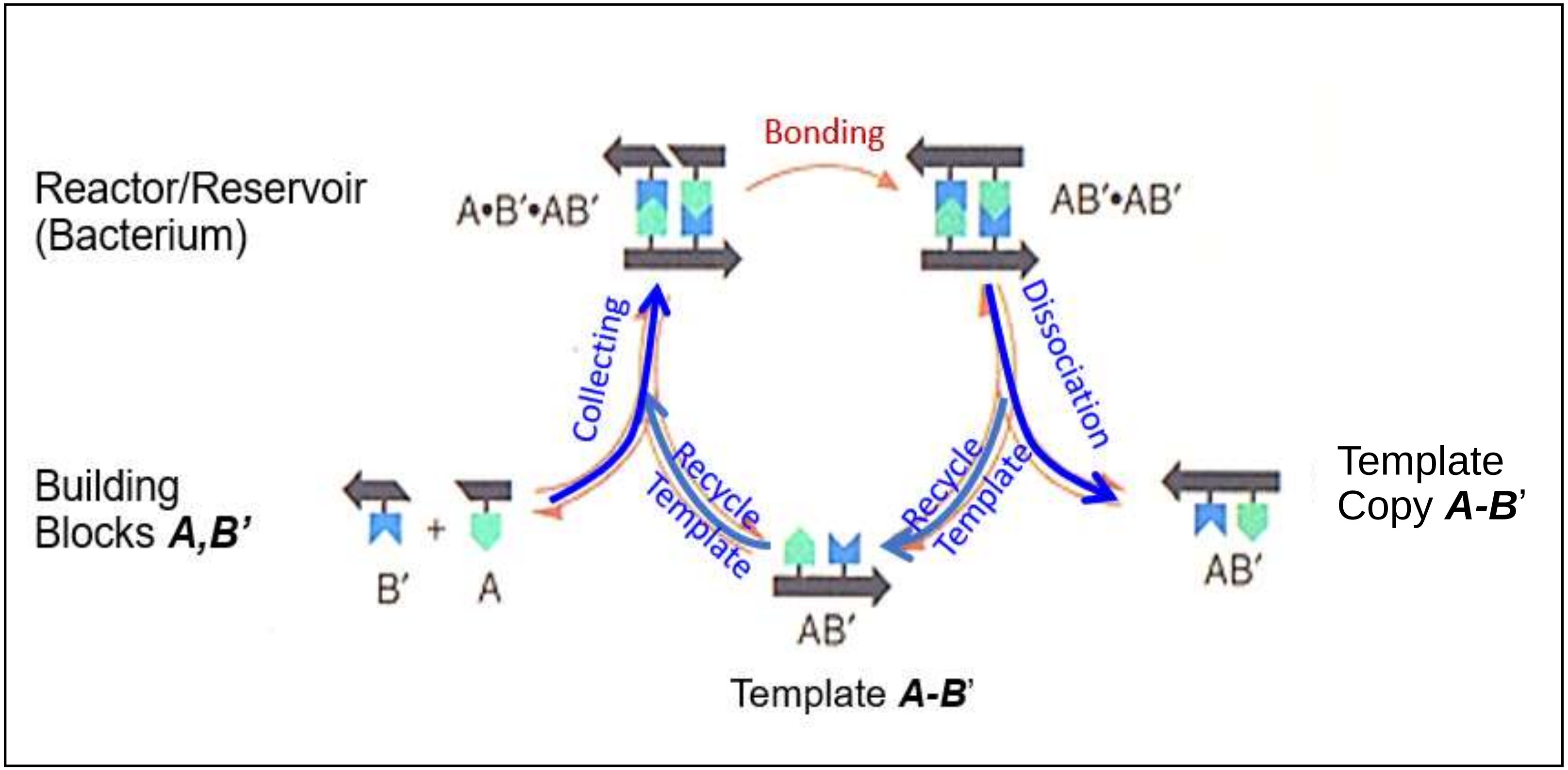
Similar oscillations: Lotka-Volterra

See computer codes in Kondepudi Ch. 19

Autocorrelation rxns

Autocatalytic Self-Replication: Schematic

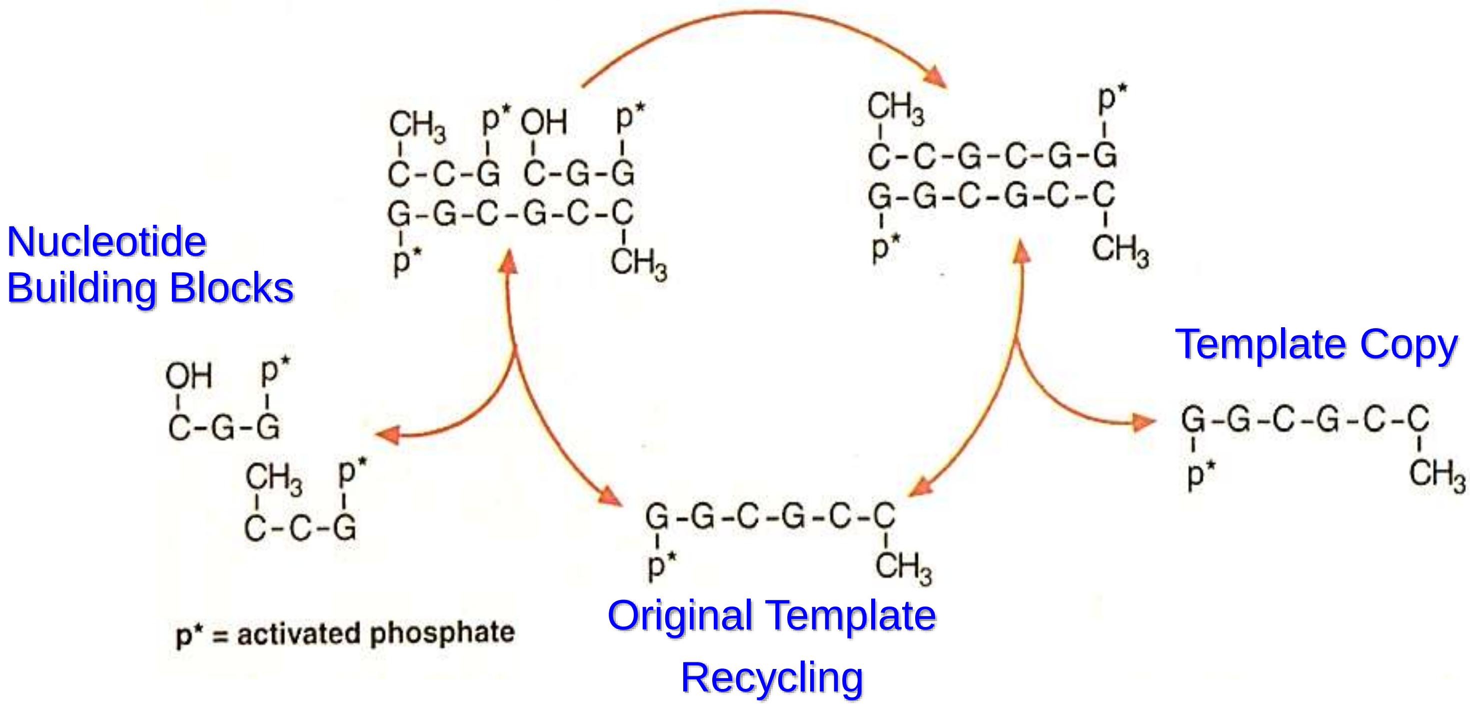
Autocatalytic self-replication with a template: Cycle attracts & combines separate building blocks *A & B'* available in environment (Reservoir) on a molecular template, dissociates template from its identical copy. Then re-cycles 2 templates in next cycle.



Each cycle makes another template copy $\Delta N / \Delta n = \lambda \cdot N(n)$ → exponential growth in numbers, inhibits/overpowers other competing processes.

Autocatalytic Self-Replication: Complementary Base-Pairing

DNA template = palindromic (left-right self-complementary)

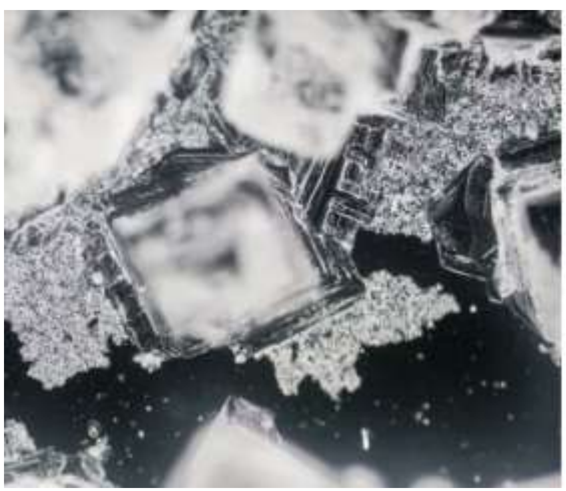


Use 2 nucleotide trimers to align and pair with hexa-DNA template, bind the two trimers → bound hexamer on template → Recover original template plus one copy.

Self-similar growth & fractal structures

Replication & Self-Similar Complexity

Manganese dendrites on limestone



Precipitate from saturated solution

Cooperative replication processes and structures to which they lead

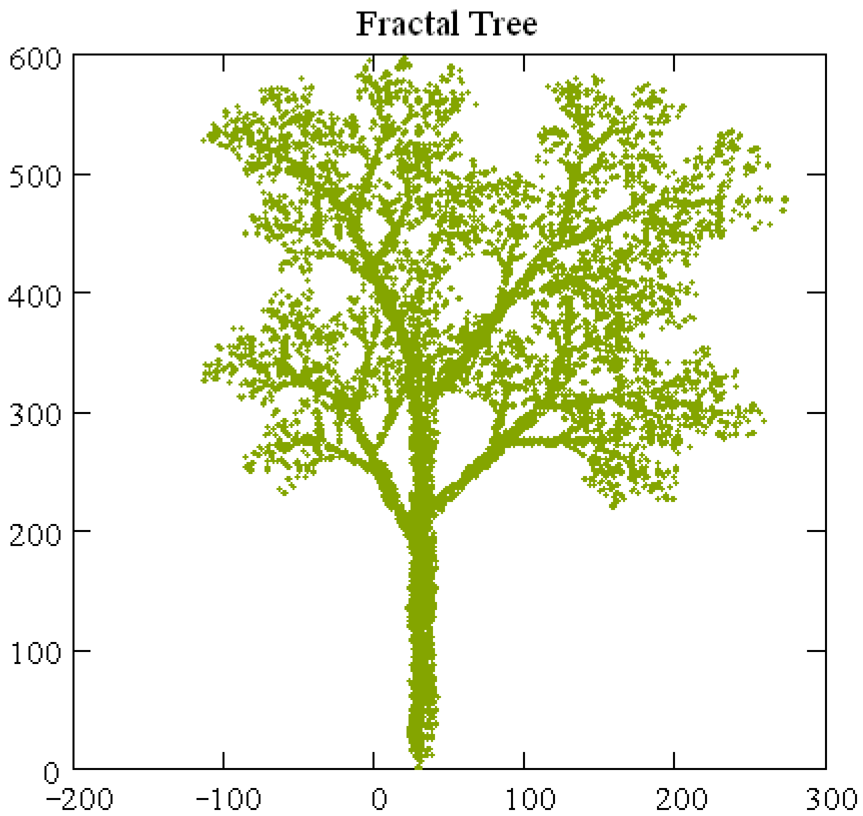
- self-organizing = (quasi-) orderly (predictable) behavior,
- co-operative growth can produce fractal structures,
- Only in the large amplitude limit (which?) complete disorder/chaos

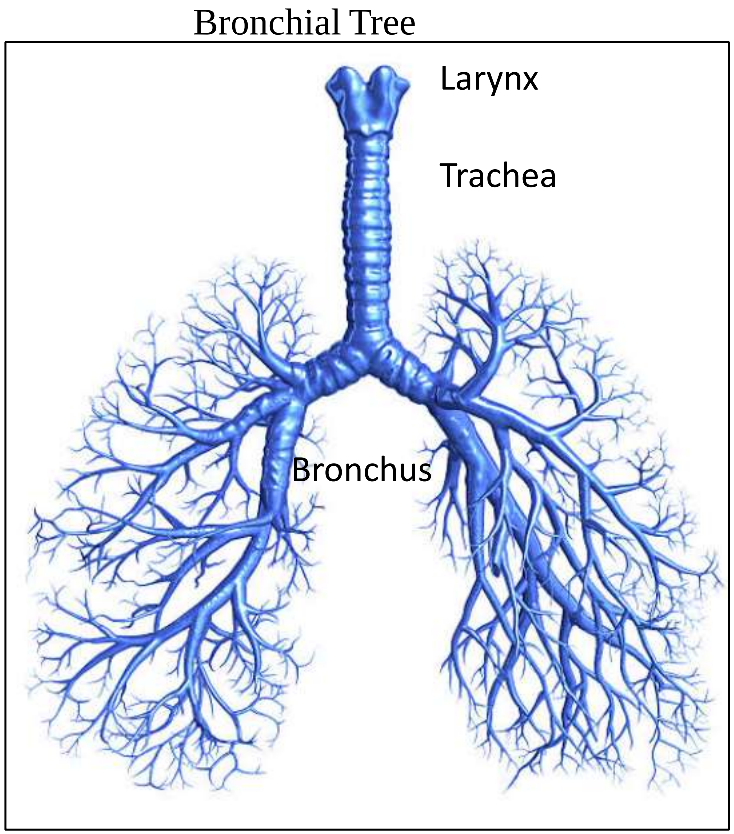
Examples:

Menger Cube d_H=2.72

- Crystallization,
- Turbulence in fluids,
- Biological life (stem cells), morphology, ageing,
- Forest fire propagation,
- Urban areal development with population growth,
- Flow patterns of electrical currents in a power grid, ….
- Behavior of gas and liquids, diffusion, convection,
- .

Self-Replication Causes Self-Similar Fractal Structures





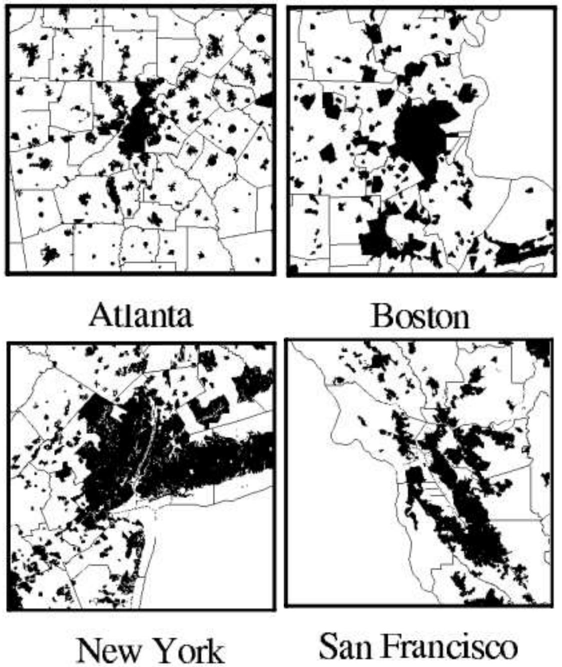
$Self - Similar\ Dynamics\ produces\ structures\ that\ repeat\ at\ different\ Scales$

$Example: Spatial\ correlation = distance\ |\vec{r}_1 - \vec{r}_2|$

$Length\ scaling\ \ factor\ L_n\ or\ L(t_n)$

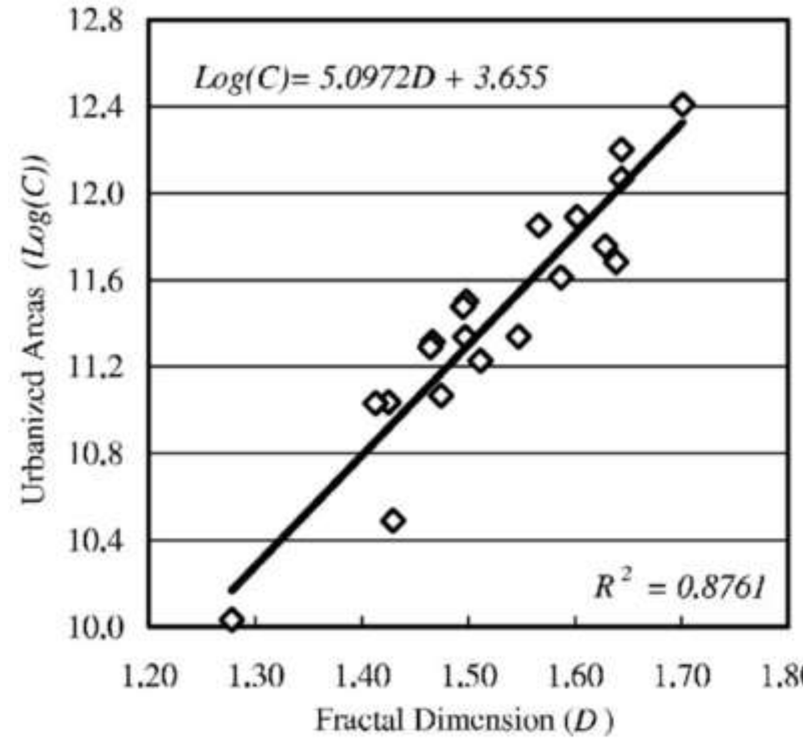
$$D_n(\vec{r}_1, \vec{r}_2) = G_n \cdot \left[\frac{f(\vec{r}_1, \vec{r}_2)}{L_n} \right]$$

Urban Growth Patterns and Forest Fires



Correlation between population size of 20 U.S. cities and occupied urban area.

Guoqiang Shen, Int. J. Geogr. Inf. Sci., 16, 419 (2002)



Forests have fractal geometry: Obvious appearance plus volume of combustible materials is related to surface area via fractal dimension → spread of forest fires.

Mathematics of Self-Replication

Represent replication structure by set of rules:

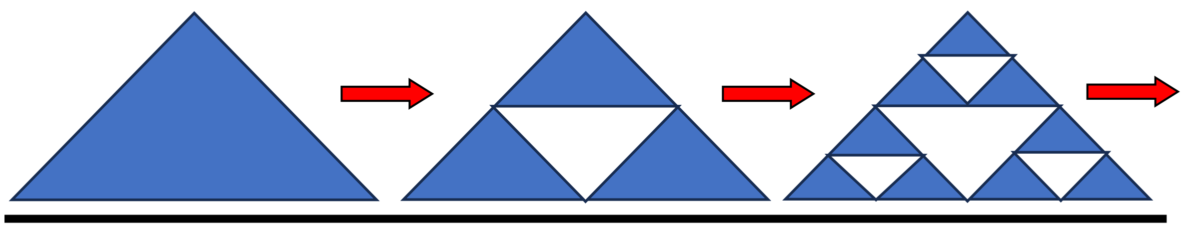
Simples case rule → function ***G***, "Parent" = Object $\boldsymbol{x = x_0}$ starting series

3-fold division ➔3 descendants $\boldsymbol{x_1 = G(x_0)}$ = 3 copies of $\boldsymbol{x_0}$ @ 1:3 scale

Possible transformation (scaling, translation, …) → Self-Similar Structures

$$x_n = \boldsymbol{G}^n(\boldsymbol{x}_0) = \boldsymbol{G}(\boldsymbol{x}_{n-1}) = \boldsymbol{G}[\boldsymbol{G}(\boldsymbol{x}_{n-2})] = \boldsymbol{G}\{\boldsymbol{G}[\boldsymbol{G}(\boldsymbol{x}_{n-3})]\} \rightarrow \textbf{Map}$$

Sierpinski Gasket

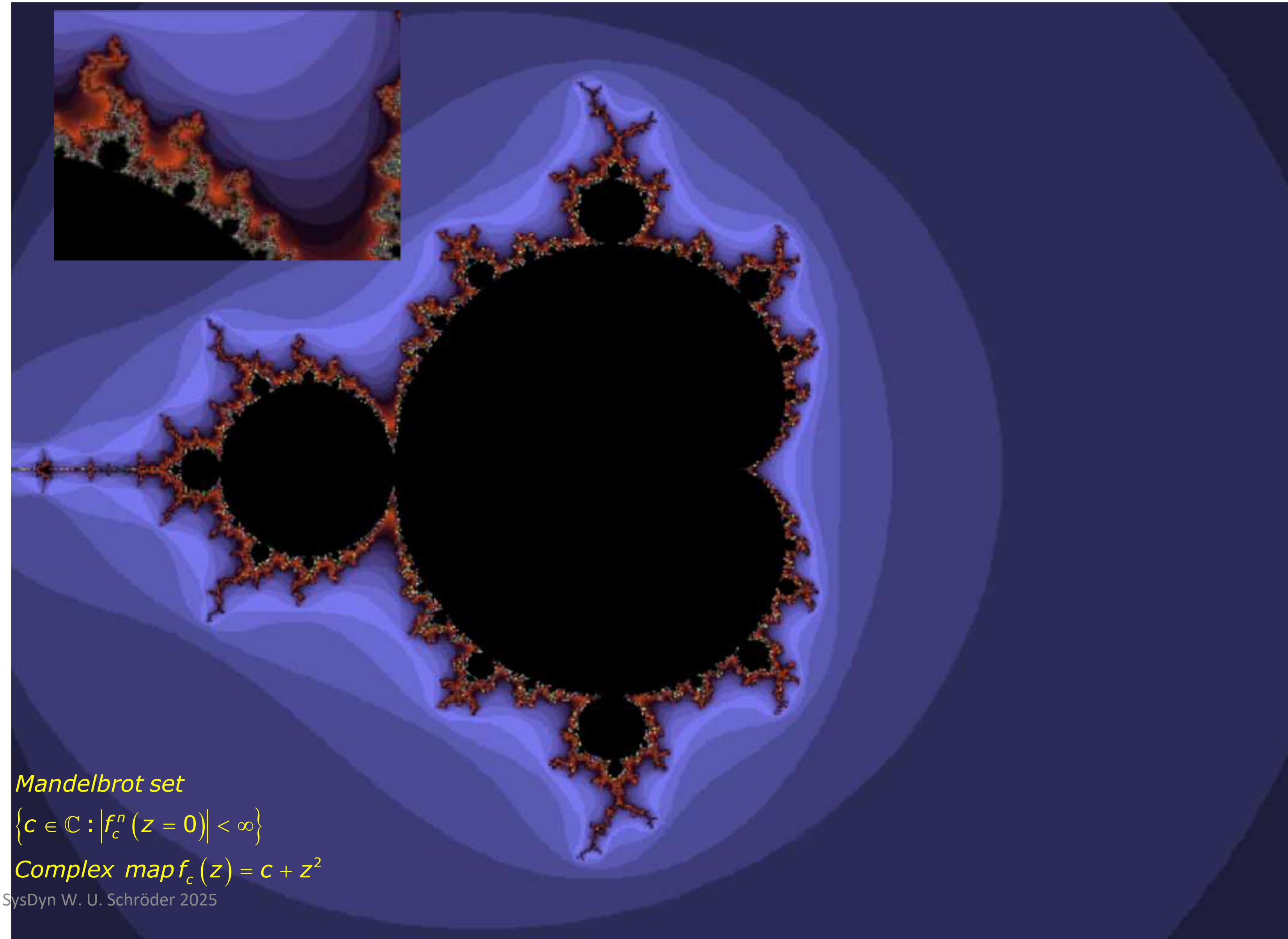


Generation $\boldsymbol{x_0}$ $\boldsymbol{x_1 = G(x_0)}$ $\boldsymbol{x_2 = G(x_1)}$

Fractal structures

See tutorial

Fractal Mandelbrot Set



Mandelbrot set

$$\left\{ c \in \mathbb{C} : \left| f_c^n \left(z = 0 \right) \right| < \infty \right\}$$

Complex map $f_c\left(z\right) = c + z^2$

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Next

Dynamics of interacting multi-particle systems
    Molecular interaction energies
    Random walk and diffusion,
    Fluctuating (Langevin) forces
    Boltzmann molecular chaos, gas laws

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Modeling Self Replicating Processes

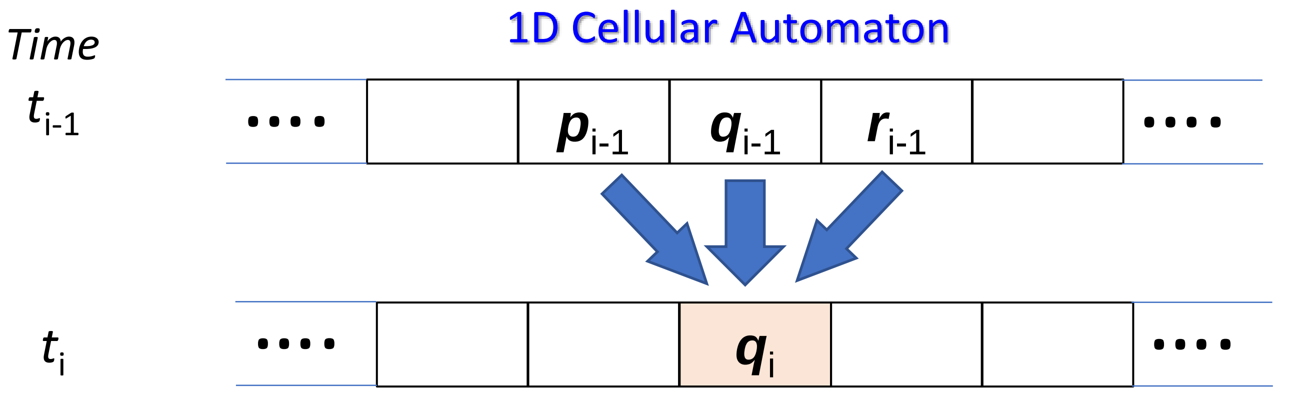
- Cellular automata (CA) are used in many fields, including physics, biology, and social science. They are computational models that simulate how patterns evolve over time
- Cellular automata have found applications in traffic modeling, with the Nagel-Schreckenberg model being a well-known example (Nagel & Schreckenberg, 1992). They have also been used to model social dynamics, epidemics, and other complex phenomena (Bagnoli, 2005).
- A CA is a collection of colored cells or atoms on a grid of a specified shape. Each cell is in one of a finite number of states. This computational model is both abstract and spatially and temporally discrete.
- There are many types of CA. The simplest type is a binary, nearest-neighbor, one-dimensional automaton called elementary cellular automata. There are 256 such CAs.
- Diffusion, corrosion, epidemics
- Cellular Automata are discrete computational systems consisting of cells that evolve in parallel at discrete time steps, inspired by self-reproducing living organisms. They are used as models of complexity, for studying nonlinear dynamics, and can compute functions and solve algorithmic problems through local interactions.

Cellular Automata-Based Modeling of Three-Dimensional Multicellular Tissue Growth, B. Ben Youssef

CA Concept

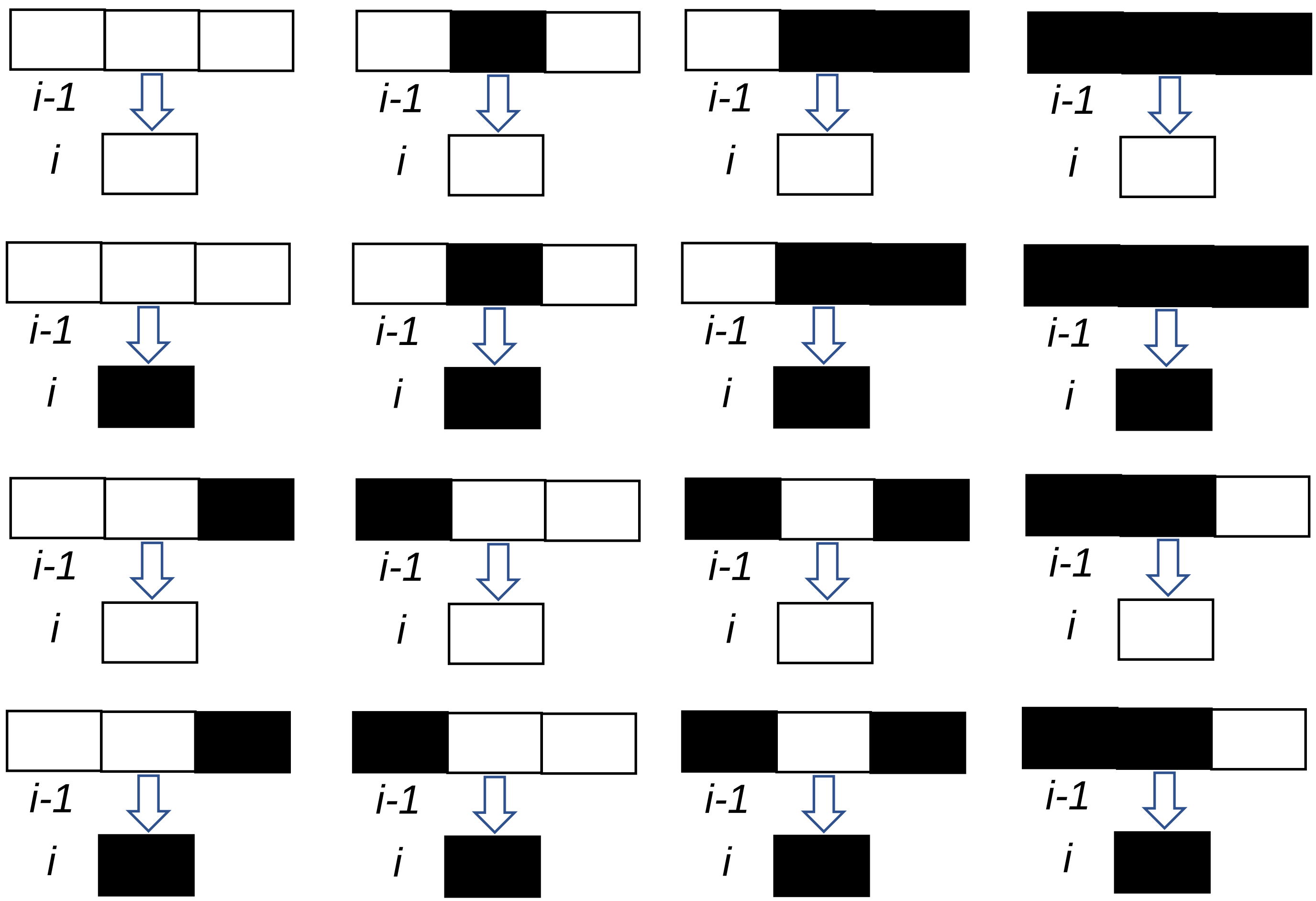
- The configuration (state) space of a system is approximated by an n-dimensional lattice of equal cells.
- Each cell has a finite number of discrete properties.
- Time evolution of CA system occurs (can be modeled) in discrete time steps → generations.
- Evolution occurs to (a set of) strict deterministic rules.
- Evolution rules reference exclusively states of neighboring cells,

  reflect local environment.



Classification of Propagation Rules

Occupied, alive | Not occupied, dead | ***Byte***



4 Rules

4 Rules

4 Rules

4 Rules

=16 Rules

Classification of Propagation Rules

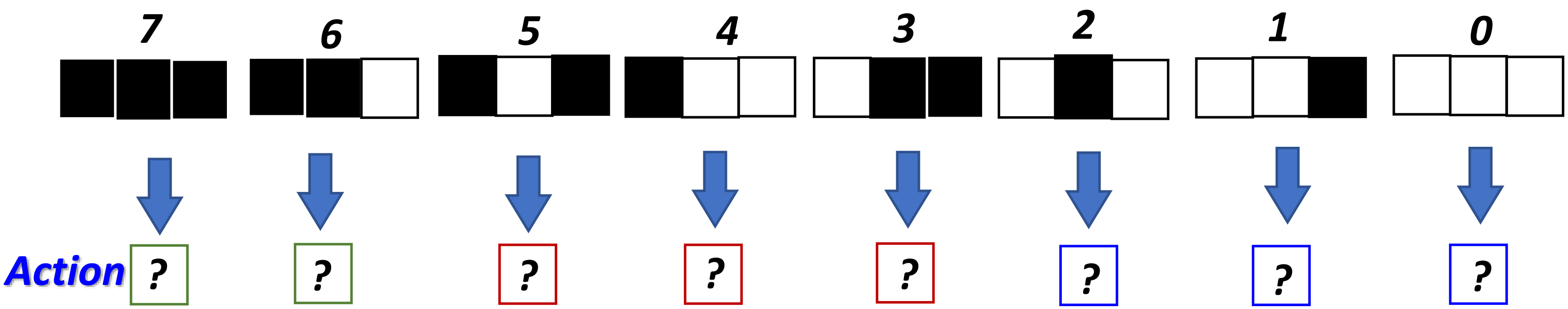
Occupied, alive

Not occupied, dead

Byte

Rearrange byte pattern in ascending order: bytes ordered in binary sequence

Condition of survival of a cell depends on the states of its own past and that of its two neighbors' past → depends on the past state of a triplet of 3 cells (=byte).



8 possible occupation patterns (≙ 0, 1, 2, 3, 4, 5, 6, 7) for each byte.
Any pattern in any one of them & ***any valid combination***, could produce an alive (= ***1***) cell or a dead (= ***0***) cell in the following time iteration step.

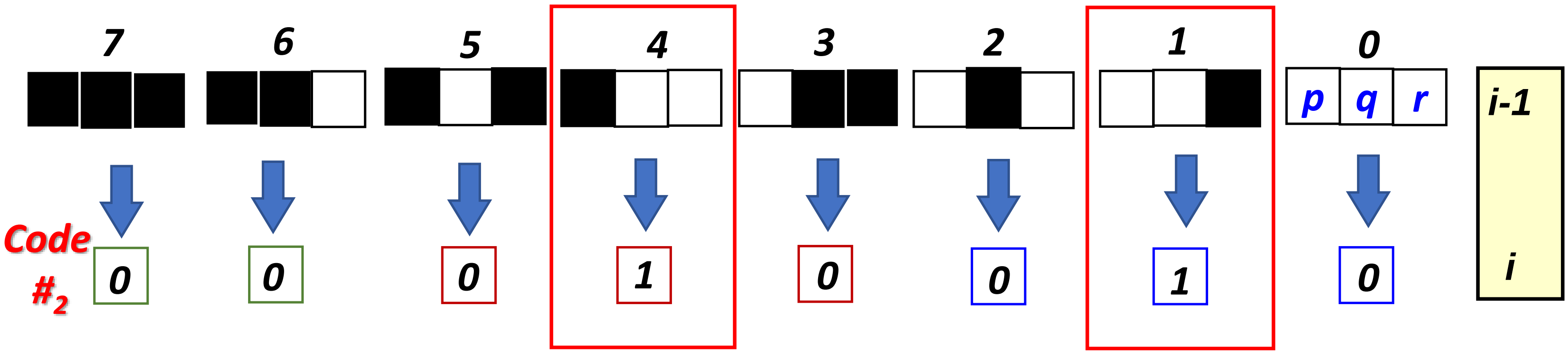
For 8 bytes, there are obviously 256 (0-255) possible conditions for an action (alive/dead). Complex preconditions for an action (0, 1) are defined by any combination (logic OR) of possible rules (represented by the set of all numbers *0,….,255*).

Classification of Propagation Rules

1 Occupied, alive **0** Not occupied, dead ***Byte***

Rearrange byte pattern in ascending order: bytes ordered in binary sequence

Condition of survival of a cell depends on the states of its own past and that of its two neighbors' past → depends on the past state of a triplet of 3 cells (=byte).



Implies live for the cell in the next time step, if it the cell was **previously unoccupied and** had only one alive neighbor on the left or on one on the right, **but not on both sides**.

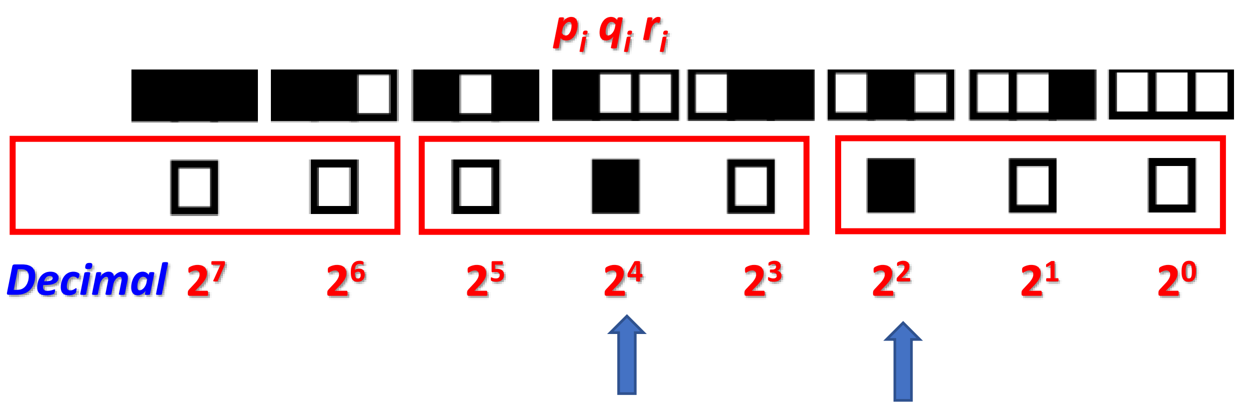
Propagation pattern

$$Code\ \#_{binary} = 10010_2 = (2^4 + 2^1) = 18_{10}$$

$$\rightarrow \boxed{q_i = (p_{i-1} \oplus r_{i-1}) \wedge (\neg q_{i-1})}$$

Interpretation of Propagation Rules

CA code # = $10100_2 = (2^4+2^2) = 20_{10}$



if (p_i) is occupied
and (q_i) is not
and (r_i) is not

if (q_i) is occupied
and (p_i) is not
and (r_i) is not

In the next time step,
center cell **(q_{i+1})** is populated

Formal logic $q_{i+1} == (p_i \oplus q_i) \wedge \neg r_i$

Truth Table $(p \wedge \neg r)$

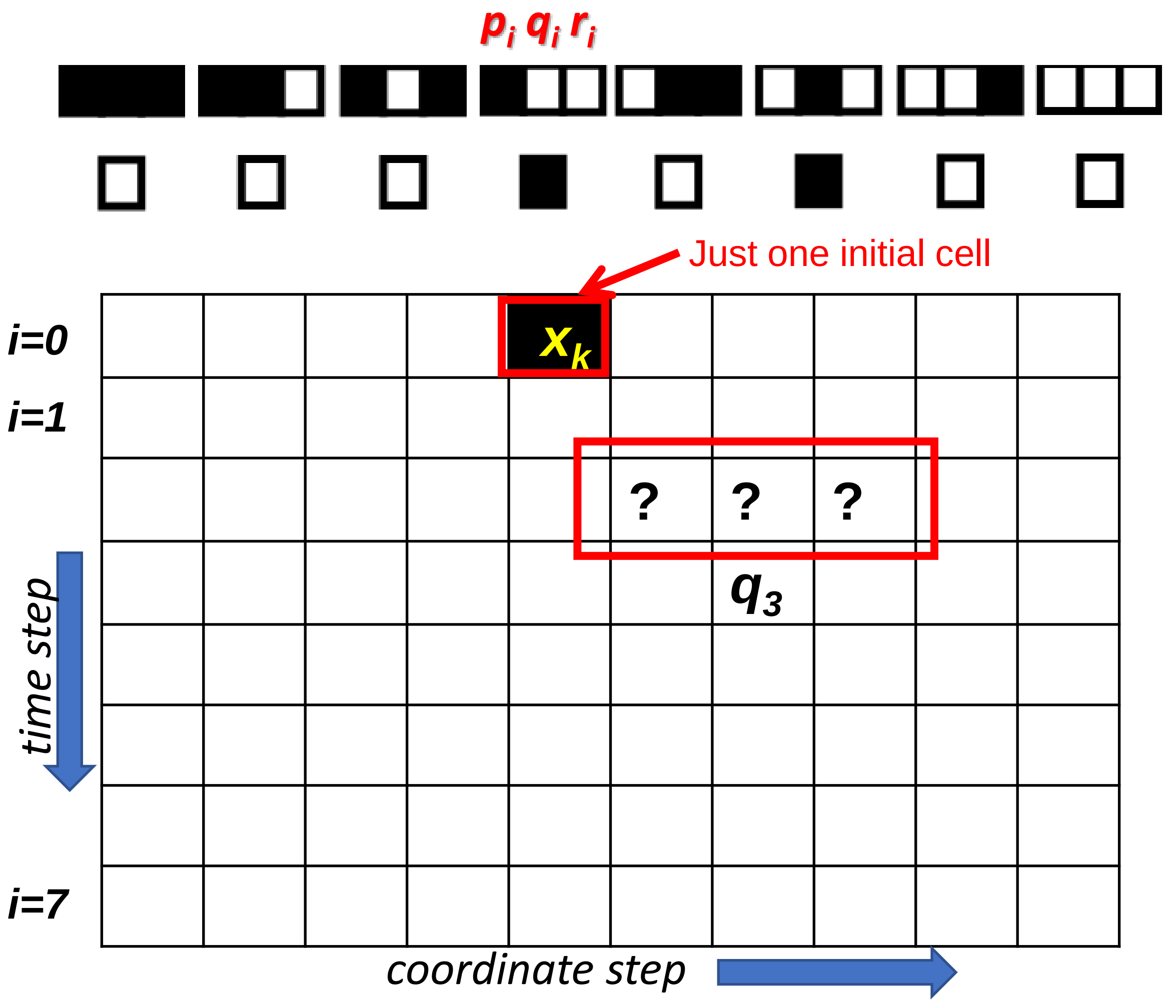
$p \backslash r$	T	F
T	F	T
F	F	F

Constructing the Propagation: CA *20*

CA code # = $10100_2 = (2^4+2^2) = 20_{10}$

Procedure

1. Draw grid
   x (k) vs. ***time (i)***
2. Load initial conditions, pattern $\boldsymbol{x_k}(i=0)$
3. Derive pattern $\boldsymbol{x_k}(i=1)$ from population of triplet $\{\boldsymbol{x_{k-1}}, \boldsymbol{x_k}, \boldsymbol{x_{k+1}},\}$ at (***i=0***)
4. Next row ***i***……
5. For self-replication, keep history



Constructing the Propagation: CA *20*

CA code # = $10100_2 = (2^4+2^2) = 20_{10}$

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4. Next row ***i***……
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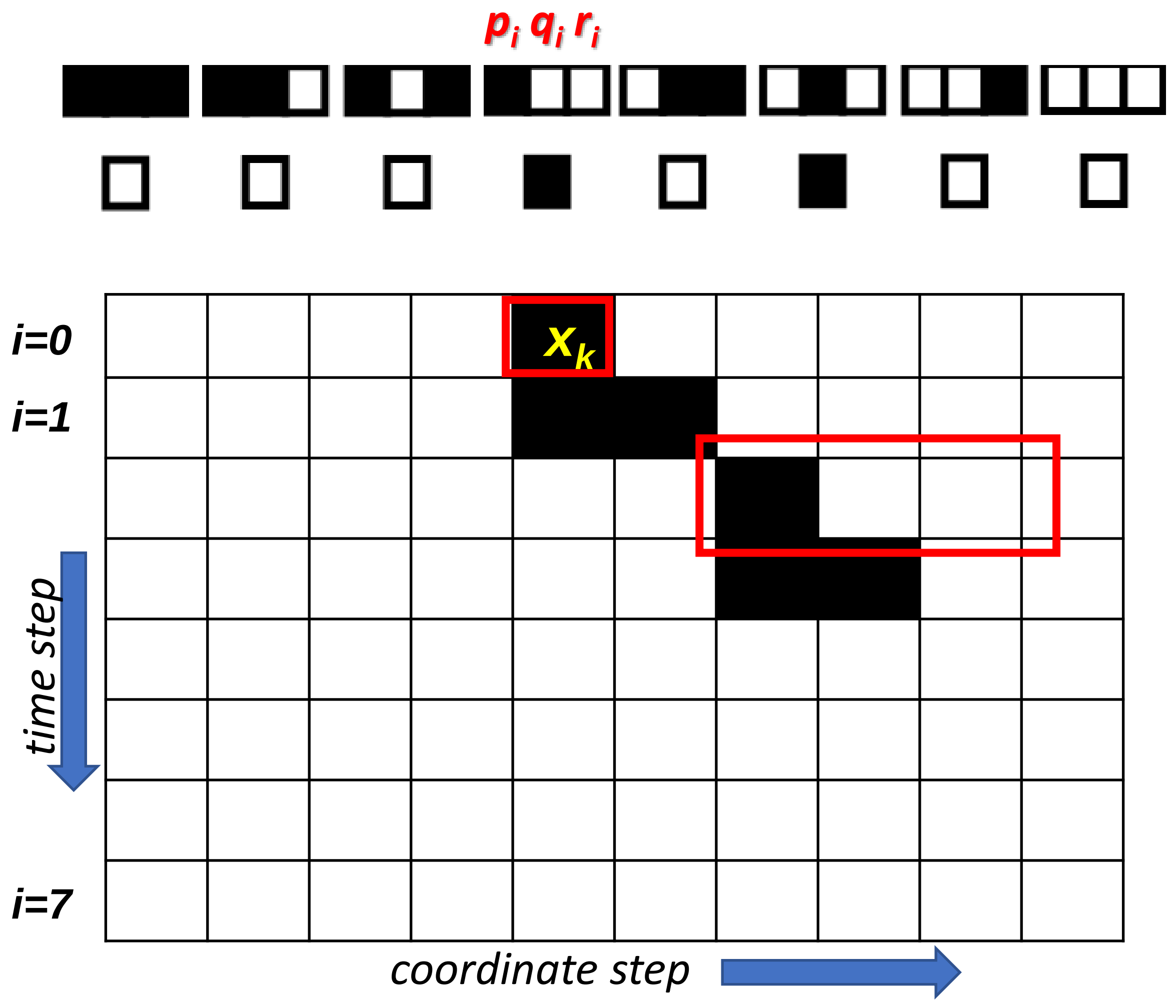
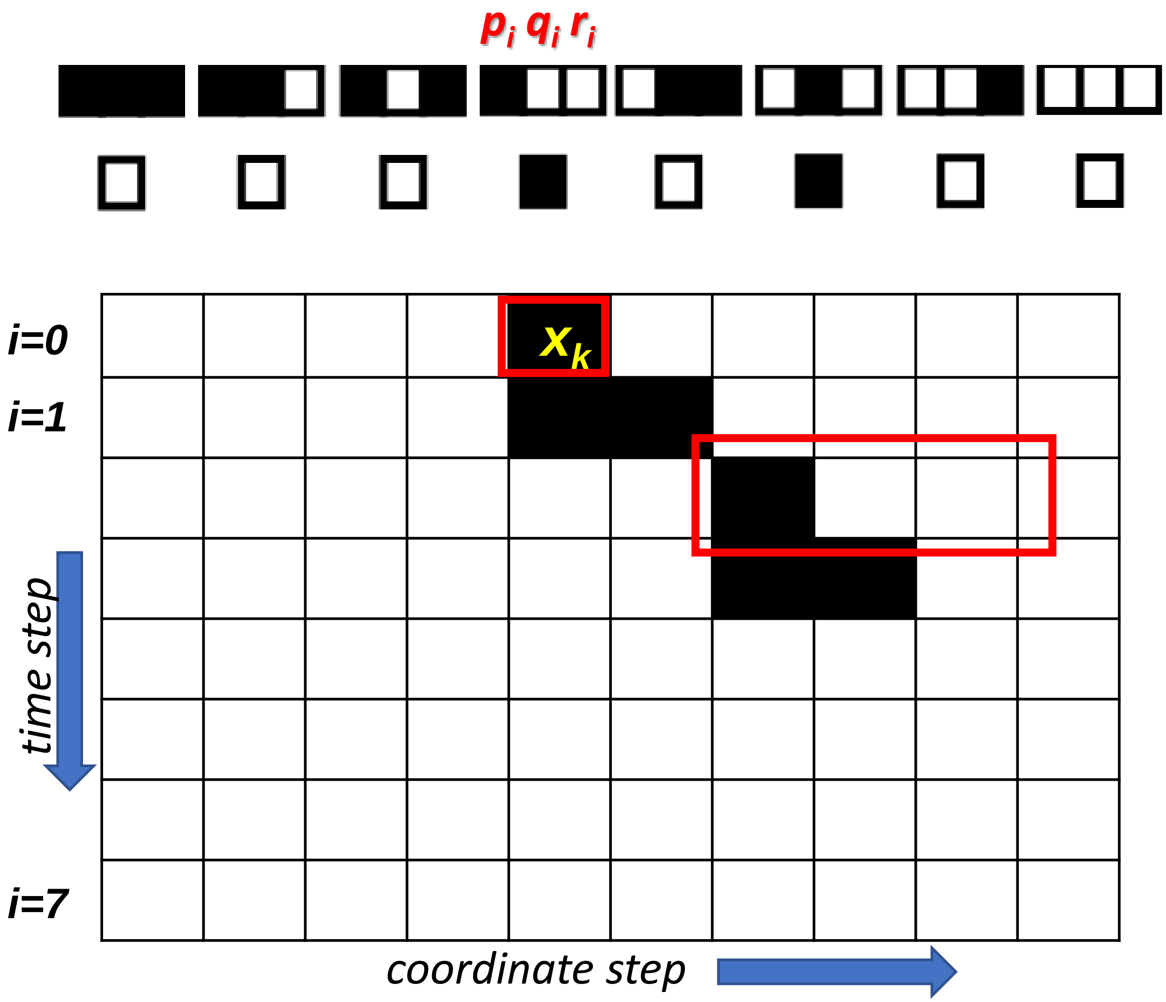


Constructing the Propagation: CA ***20***

CA code # = $10100_2 = (2^4+2^2) = 20_{10}$

Procedure

1. Draw grid
   x (k) vs. ***time (i)***
2. Load initial conditions, pattern $x_k(i=0)$
3. Derive pattern $x_k(i=1)$ from population of triplet $\{x_{k-1}, x_k, x_{k+1}\}$ at ($i=0$)
4. Next row ***i***……
5. For self-replication, keep history



Coding CA#20

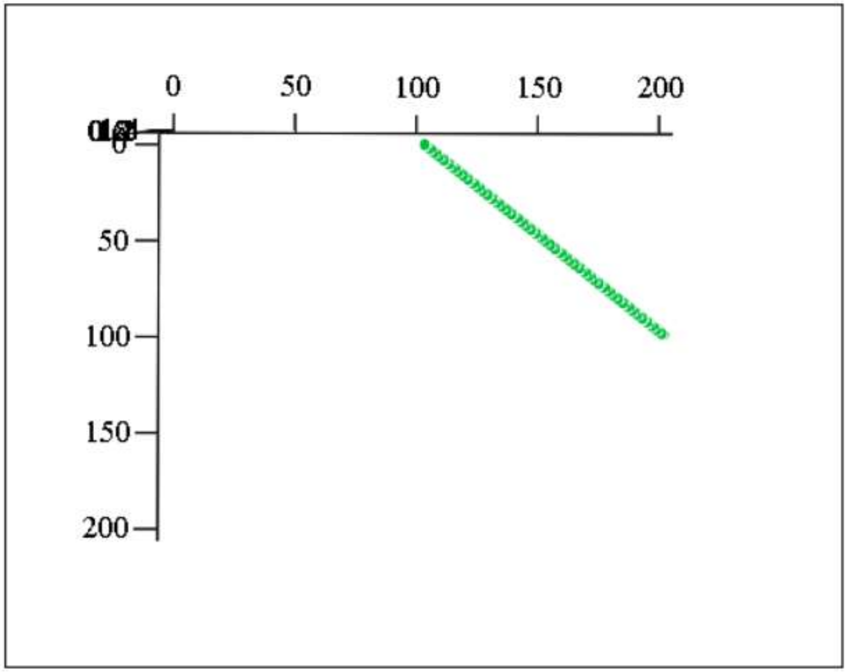
Data: Either single valued initial condition or random with different intensity chosen by width of acceptance window for r
Rule numbers according to Stephen Wolfram (A New
Science , Wolfram Media, 2002

$N := 200$ Data: Array size in x (N) and number of it

$M := 200$

$i := 1 .. N$

$j := 1 .. M$



$A_{i,j} := 0$ Initial values

$A_{0,100} := 1$

$j := 1 .. M - 1$

Rule 20: (p Xor q) and not r

$$A_{i,j} := \begin{array}{|l} a \leftarrow 0 \\ p \leftarrow A_{i-1,j-1} \\ q \leftarrow A_{i-1,j} \\ r \leftarrow A_{i-1,j+1} \\ a \leftarrow 1 \ \text{ if } (p = 1 \oplus q = 1) \wedge [\neg(r = 1)] \\ a \end{array}$$

Coding CA#30

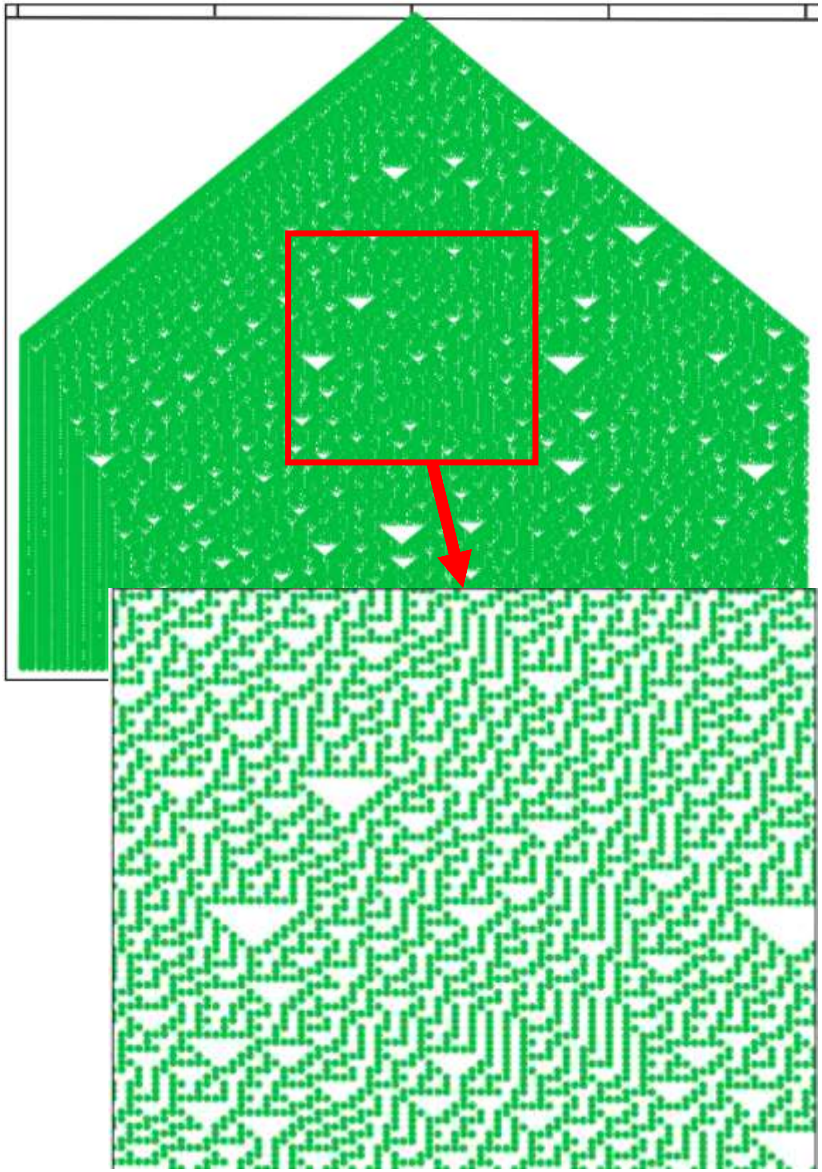
$A_{i,j} := 0$

$A_{0,100} := 1$ Initial values 1,0 +

$j := 1..M-1$

Rule 30: p Xor (q or r)
random

$$A_{i,j} := \left| \begin{array}{l} a \leftarrow 0 \\ p \leftarrow A_{i-1,j-1} \\ q \leftarrow A_{i-1,j} \\ r \leftarrow A_{i-1,j+1} \\ a \leftarrow 1 \quad \text{if } p = 1 \oplus (q = 1 \vee r = 1) \\ a \end{array} \right.$$



CA #30, with one more condition. More complex pattern. Repetitive fine structure is observed at the rim of the triangle and upon blowup.

Coding CA#90 Specific IC

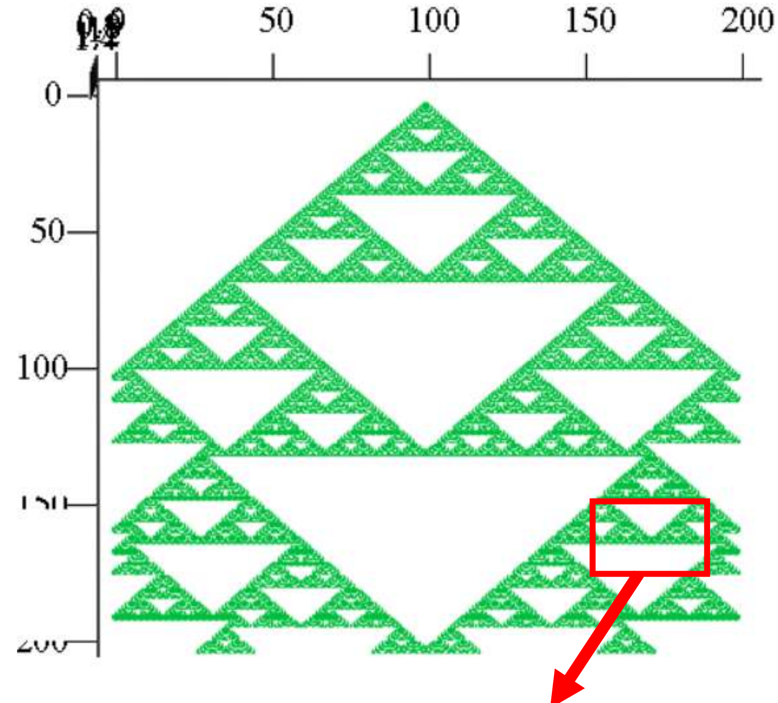
$A_{i,j} := 0$

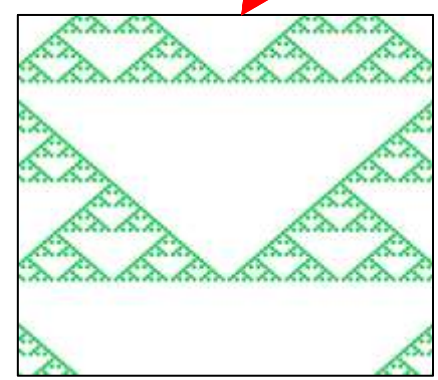
$A_{0,100} := 1$ Initial values 1,0

$j := 1..M-1$

$$A_{i,j} := \left| \begin{array}{l} a \leftarrow 0 \\ p \leftarrow A_{i-1,j-1} \\ q \leftarrow A_{i-1,j} \\ r \leftarrow A_{i-1,j+1} \\ a \leftarrow 1 \ \text{ if } (p = 1) \oplus (r = 1) \\ a \end{array} \right.$$

Rule 90: p Xor r
fractal structure





CA #90, could be expected to show similar randomness as automaton #30. Instead, a highly repetitive pattern of nested triangles results. Blow-up: persists at several length scales (self-similar/fractal).

Coding CA#90 Specific Initial Conditions

$A_{i,j} := 0$

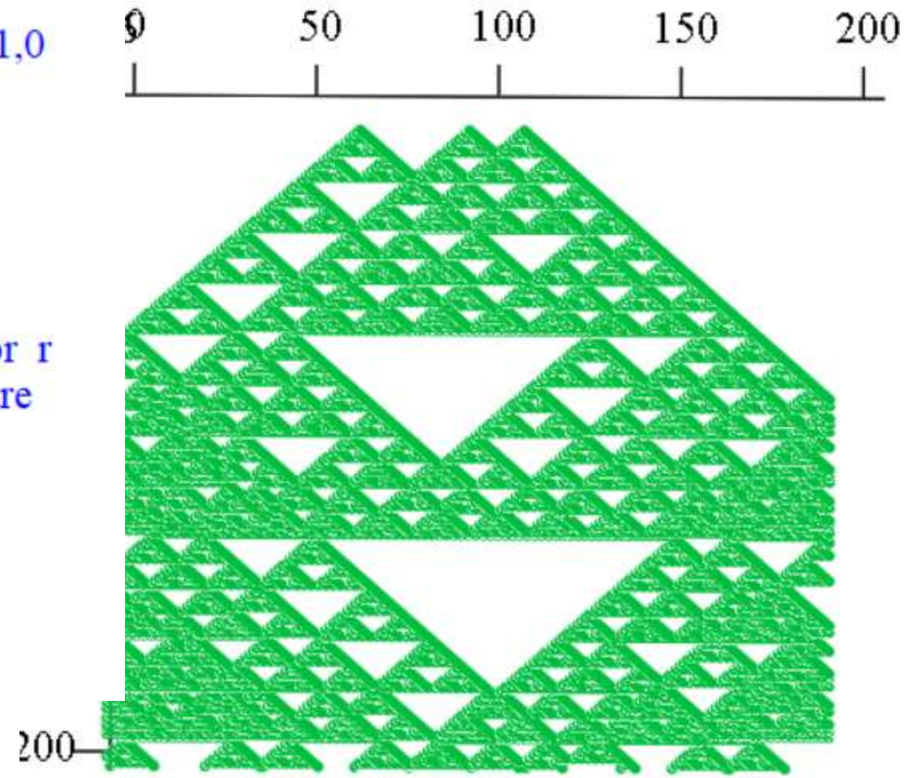
$A_{0,100} := 1$ Initial values 1,0

$A_{0,70} := 1 \quad A_{0,110} := 1$

$j := 1..M-1$

$$A_{i,j} := \left| \begin{array}{l} a \leftarrow 0 \\ p \leftarrow A_{i-1,j-1} \\ q \leftarrow A_{i-1,j} \\ r \leftarrow A_{i-1,j+1} \\ a \leftarrow 1 \;\; \text{if } (p = 1) \oplus (r = 1) \\ a \end{array} \right.$$

Rule 90: p Xor r
fractal structure



CA #90, with 3 initial cells populated.
Fractal structure is modified but persists.

Coding CA#90 Random IC

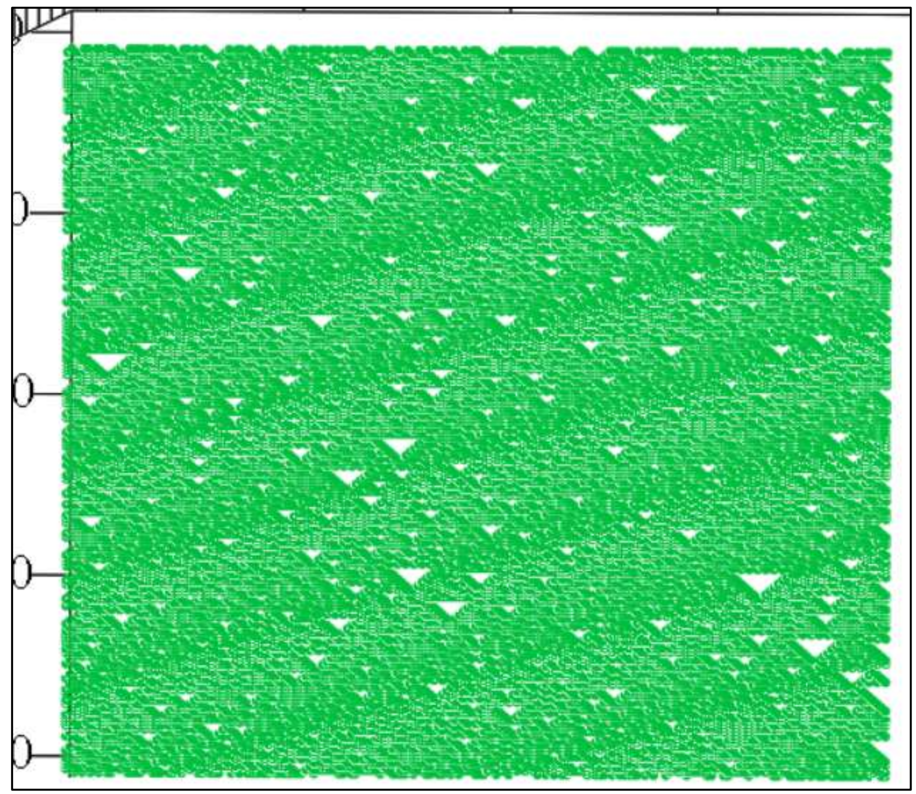
$A_{0,j} := \begin{cases} 0 \\ 1 \;\; \text{if } \text{rnd}(1) > 0.5 \end{cases}$ Random initial values 1,0

$j := 1..M-1$

$$A_{i,j} := \begin{array}{|l} a \leftarrow 0 \\ p \leftarrow A_{i-1,j-1} \\ q \leftarrow A_{i-1,j} \\ r \leftarrow A_{i-1,j+1} \\ a \leftarrow 1 \;\; \text{if } (p = 1) \oplus (r = 1) \\ a \end{array}$$

Rule 90: p Xor r
fractal structure

CA #90, with random population of 50% of initial cells.
Specific fractal structure is washed out, additional pattern appears on larger length scale.



Approximates Random chaos

Summary

CA research: 4 classes of automata,

- Class 1 reaches a homogeneous state (all cells free) after a few initial steps.
- Class 2 shows a periodic pattern after the first few steps, relatively independent of initial conditions.
- Class 3 develops into a chaotic pattern, independent of initial conditions.
- Class 4 produces a highly complex, nested fractal pattern.

Very specific, simple, localized microscopic interactions of coupled systems can lead to highly organized structure.

Pronounced fractal structure emerges from localized initial conditions (seeds).

Spread-out initial state conditions lead to washed out structures or chaos.

Because of their specific (unusual) geometrical shape (surface/volume), Class-4

CAs have functionality important for live, biomed and general technology.

Fractal dimensions